



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 12:36 AM UTC

PDB ID : 2C8H / pdb_00002c8h
Title : Structure of the PN loop Q182A mutant C3bot1 Exoenzyme (NAD-bound state, crystal form I)
Authors : Stura, E.A.; Menetrey, J.; Flatau, G.; Boquet, P.; Menez, A.
Deposited on : 2005-12-03
Resolution : 1.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

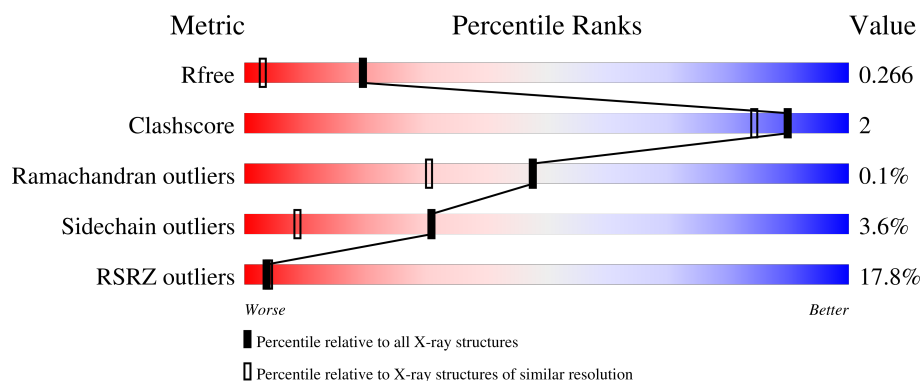
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	211	7% 93% • •
1	B	211	23% 88% 8% • •
1	C	211	22% 90% 9% •
1	D	211	17% 91% 6% •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7257 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called MONO-ADP-RIBOSYLTRANSFERASE C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	204	Total	C	N	O	S	4	0	0
			1598	1015	272	304	7			
1	B	205	Total	C	N	O	S	24	0	0
			1606	1021	273	305	7			
1	C	208	Total	C	N	O	S	9	0	0
			1626	1034	277	308	7			
1	D	204	Total	C	N	O	S	10	0	0
			1595	1014	271	303	7			

There are 4 discrepancies between the modelled and reference sequences:

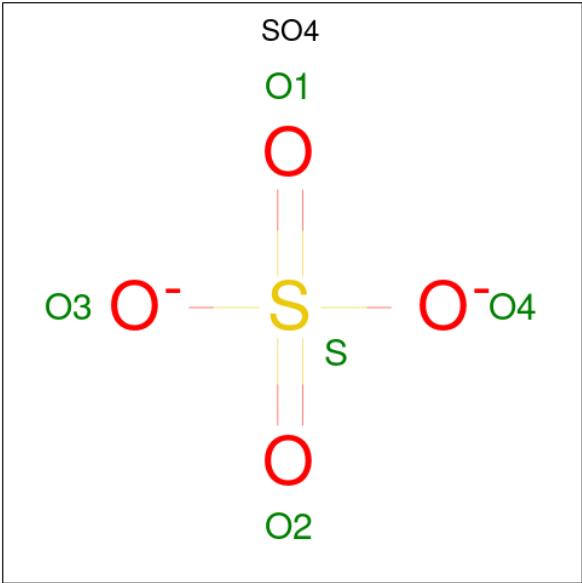
Chain	Residue	Modelled	Actual	Comment	Reference
A	182	ALA	GLN	engineered mutation	UNP P15879
B	182	ALA	GLN	engineered mutation	UNP P15879
C	182	ALA	GLN	engineered mutation	UNP P15879
D	182	ALA	GLN	engineered mutation	UNP P15879

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	B	1	Total 44	C 21	N 7	O 14	P 2	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

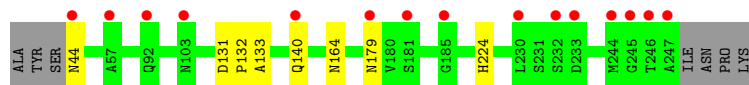
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	230	Total	O	0	0
			230	230		
4	B	147	Total	O	0	0
			147	147		
4	C	157	Total	O	0	0
			157	157		
4	D	180	Total	O	0	0
			180	180		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

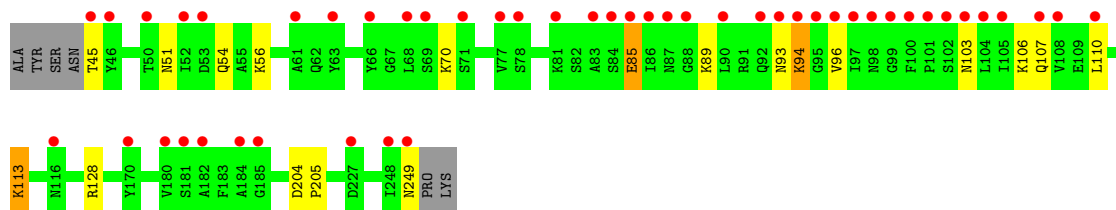
• Molecule 1: MONO-ADP-RIBOSYLTRANSFERASE C3

Chain A: 

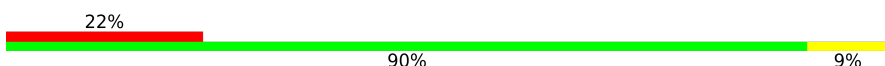


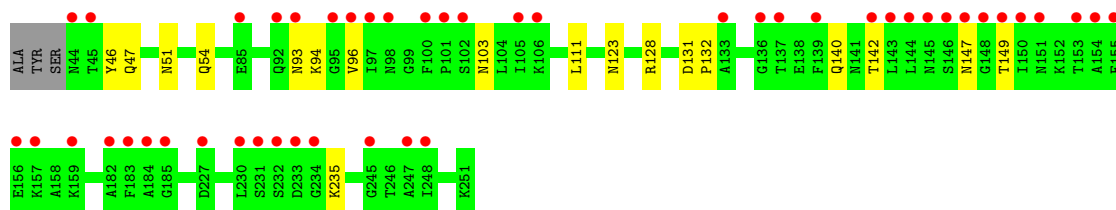
• Molecule 1: MONO-ADP-RIBOSYLTRANSFERASE C3

Chain B: 



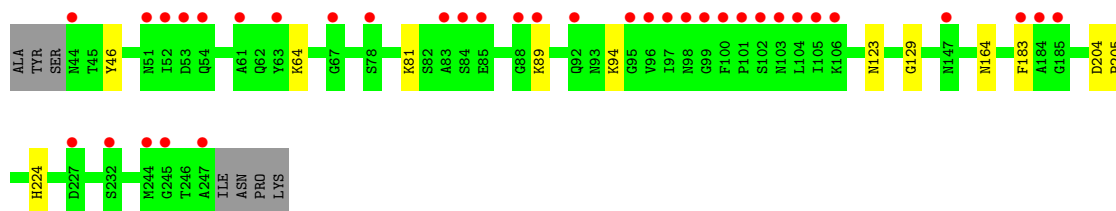
• Molecule 1: MONO-ADP-RIBOSYLTRANSFERASE C3

Chain C: 



• Molecule 1: MONO-ADP-RIBOSYLTRANSFERASE C3

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	105.39Å 75.61Å 120.78Å 90.00° 102.75° 90.00°	Depositor
Resolution (Å)	31.78 – 1.65 31.78 – 1.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (31.78-1.65) 96.7 (31.78-1.65)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.216 , 0.259 0.223 , 0.266	Depositor DCC
R_{free} test set	5365 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	24.9	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 36.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7257	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, NAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.45	0/1626	0.70	0/2184
1	B	0.49	1/1634 (0.1%)	0.75	1/2195 (0.0%)
1	C	0.50	1/1655 (0.1%)	0.75	0/2224
1	D	0.45	0/1623	0.74	0/2180
All	All	0.47	2/6538 (0.0%)	0.74	1/8783 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	103	ASN	CA-CB	-6.89	1.42	1.53
1	B	85	GLU	CB-CG	-5.99	1.34	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	85	GLU	CA-CB-CG	5.62	125.35	114.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1598	0	1618	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1606	0	1629	9	0
1	C	1626	0	1646	5	0
1	D	1595	0	1614	5	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
3	A	10	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	10	0	0	0	0
4	A	230	0	0	1	0
4	B	147	0	0	0	0
4	C	157	0	0	0	0
4	D	180	0	0	0	0
All	All	7257	0	6559	23	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (23) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:ASN:HD21	1:C:54:GLN:HE21	1.25	0.83
1:C:51:ASN:HD21	1:C:54:GLN:NE2	1.97	0.63
1:D:129:GLY:HA3	1:D:183:PHE:HB2	1.81	0.62
1:B:93:ASN:O	1:B:96:VAL:HG22	2.02	0.60
1:A:133:ALA:HB2	1:A:140:GLN:NE2	2.18	0.58
1:B:94:LYS:O	1:B:94:LYS:HG2	2.03	0.58
1:B:110:LEU:HD23	1:B:113:LYS:NZ	2.19	0.57
1:B:94:LYS:O	1:B:94:LYS:CG	2.58	0.52
1:A:133:ALA:HB2	1:A:140:GLN:HE22	1.77	0.49
1:A:164:ASN:OD1	1:A:224:HIS:HE1	1.96	0.49
4:A:2142:HOH:O	1:B:249:ASN:C	2.59	0.46
1:D:164:ASN:OD1	1:D:224:HIS:HE1	2.01	0.44
1:D:164:ASN:OD1	1:D:224:HIS:CE1	2.70	0.44
1:C:46:TYR:CD1	1:C:123:ASN:HB3	2.53	0.44
1:A:131:ASP:HB3	1:A:132:PRO:CD	2.48	0.43
1:B:51:ASN:HD21	1:B:54:GLN:HB2	1.83	0.43
1:D:204:ASP:N	1:D:205:PRO:CD	2.82	0.42
1:B:110:LEU:HD23	1:B:113:LYS:HZ1	1.83	0.42
1:B:204:ASP:N	1:B:205:PRO:CD	2.83	0.41
1:D:46:TYR:CD1	1:D:123:ASN:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:ASP:HB3	1:C:132:PRO:CD	2.51	0.41
1:B:110:LEU:HD23	1:B:113:LYS:HZ3	1.85	0.40
1:C:149:THR:HA	1:C:235:LYS:HA	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	202/211 (96%)	200 (99%)	2 (1%)	0	100	100
1	B	203/211 (96%)	200 (98%)	3 (2%)	0	100	100
1	C	206/211 (98%)	200 (97%)	5 (2%)	1 (0%)	24	10
1	D	202/211 (96%)	201 (100%)	1 (0%)	0	100	100
All	All	813/844 (96%)	801 (98%)	11 (1%)	1 (0%)	48	30

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	147	ASN

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	172/178 (97%)	170 (99%)	2 (1%)	63	45
1	B	173/178 (97%)	162 (94%)	11 (6%)	16	3
1	C	174/178 (98%)	166 (95%)	8 (5%)	24	5
1	D	171/178 (96%)	167 (98%)	4 (2%)	44	21
All	All	690/712 (97%)	665 (96%)	25 (4%)	31	9

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	179	ASN
1	B	45	THR
1	B	56	LYS
1	B	70	LYS
1	B	85	GLU
1	B	89	LYS
1	B	94	LYS
1	B	103	ASN
1	B	106	LYS
1	B	107	GLN
1	B	113	LYS
1	B	128	ARG
1	C	47	GLN
1	C	93	ASN
1	C	94	LYS
1	C	96	VAL
1	C	111	LEU
1	C	128	ARG
1	C	140	GLN
1	C	142	THR
1	D	64	LYS
1	D	81	LYS
1	D	89	LYS
1	D	94	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	ASN
1	A	140	GLN

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Mol	Chain	Res	Type
1	A	141	ASN
1	A	224	HIS
1	B	47	GLN
1	B	51	ASN
1	B	107	GLN
1	B	140	GLN
1	B	212	GLN
1	B	224	HIS
1	C	54	GLN
1	C	93	ASN
1	C	98	ASN
1	C	107	GLN
1	C	224	HIS
1	C	236	GLN
1	D	62	GLN
1	D	224	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	B	1250	-	46,48,48	1.74	7 (15%)	64,73,73	1.65	10 (15%)
3	SO4	A	1249	-	4,4,4	0.24	0	6,6,6	0.16	0
3	SO4	D	1249	-	4,4,4	0.26	0	6,6,6	0.06	0
3	SO4	C	1252	-	4,4,4	0.24	0	6,6,6	0.09	0
3	SO4	D	1248	-	4,4,4	0.22	0	6,6,6	0.17	0
3	SO4	B	1251	-	4,4,4	0.25	0	6,6,6	0.20	0
2	NAD	A	1248	-	46,48,48	1.60	5 (10%)	64,73,73	1.58	9 (14%)
3	SO4	A	1250	-	4,4,4	0.25	0	6,6,6	0.09	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	A	1248	-	-	3/30/62/62	0/5/5/5
2	NAD	B	1250	-	-	6/30/62/62	0/5/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1250	NAD	O7N-C7N	8.87	1.40	1.24
2	A	1248	NAD	O7N-C7N	8.16	1.39	1.24
2	A	1248	NAD	C2A-N3A	2.79	1.38	1.33
2	B	1250	NAD	C2A-N1A	2.75	1.38	1.33
2	B	1250	NAD	C2N-N1N	2.73	1.38	1.35
2	B	1250	NAD	C2A-N3A	2.72	1.38	1.33
2	B	1250	NAD	PN-O3	2.70	1.62	1.59
2	A	1248	NAD	C2A-N1A	2.63	1.38	1.33
2	A	1248	NAD	C2N-N1N	2.32	1.37	1.35
2	B	1250	NAD	PA-O3	2.29	1.62	1.59
2	A	1248	NAD	C8A-N7A	2.26	1.36	1.31
2	B	1250	NAD	C8A-N7A	2.01	1.35	1.31

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1250	NAD	N3A-C2A-N1A	-5.52	120.23	128.58
2	A	1248	NAD	N3A-C2A-N1A	-5.35	120.48	128.58
2	B	1250	NAD	C5A-C4A-N3A	-4.53	120.48	126.72
2	A	1248	NAD	C3N-C7N-N7N	4.44	123.22	117.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1250	NAD	C3N-C7N-N7N	4.18	122.88	117.74
2	A	1248	NAD	C5A-C4A-N3A	-4.16	120.99	126.72
2	B	1250	NAD	N9A-C8A-N7A	-3.80	108.55	113.94
2	A	1248	NAD	N9A-C8A-N7A	-3.77	108.58	113.94
2	B	1250	NAD	C5A-N7A-C8A	3.43	108.84	103.45
2	B	1250	NAD	C2A-N3A-C4A	3.43	120.21	111.83
2	A	1248	NAD	C5A-N7A-C8A	3.29	108.62	103.45
2	A	1248	NAD	C2A-N3A-C4A	3.18	119.59	111.83
2	B	1250	NAD	N3A-C4A-N9A	2.94	132.16	127.17
2	A	1248	NAD	N3A-C4A-N9A	2.50	131.42	127.17
2	A	1248	NAD	O7N-C7N-C3N	-2.43	116.62	119.60
2	A	1248	NAD	C4A-C5A-N7A	-2.43	107.81	110.58
2	B	1250	NAD	C4A-C5A-N7A	-2.37	107.87	110.58
2	B	1250	NAD	C6N-N1N-C2N	-2.32	119.90	121.88
2	B	1250	NAD	O4B-C1B-N9A	2.07	112.06	108.09

There are no chirality outliers.

All (9) torsion outliers are listed below:

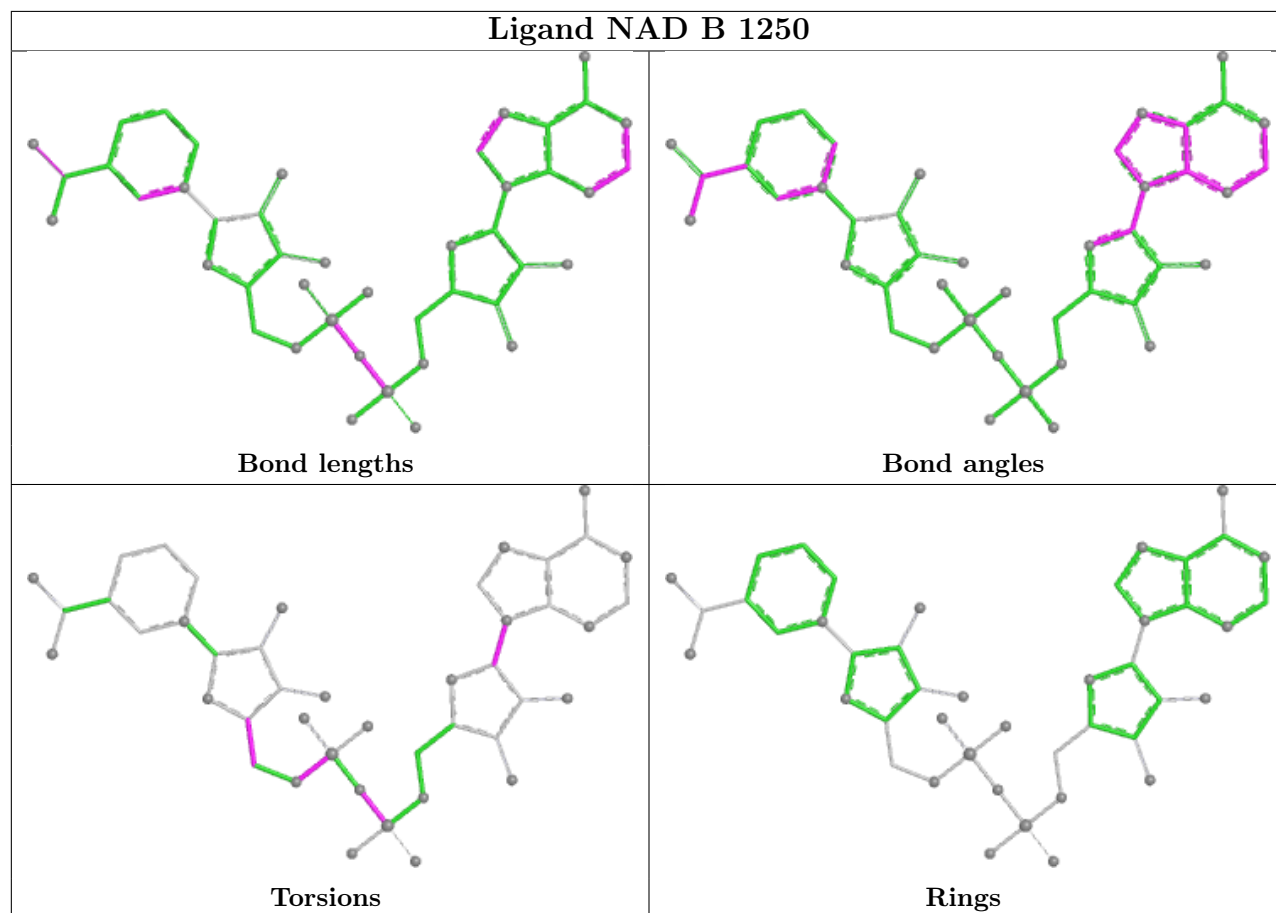
Mol	Chain	Res	Type	Atoms
2	B	1250	NAD	PN-O3-PA-O5B
2	B	1250	NAD	O4D-C4D-C5D-O5D
2	B	1250	NAD	C3D-C4D-C5D-O5D
2	A	1248	NAD	C2B-C1B-N9A-C8A
2	B	1250	NAD	C5D-O5D-PN-O1N
2	B	1250	NAD	C2B-C1B-N9A-C8A
2	A	1248	NAD	C2B-C1B-N9A-C4A
2	A	1248	NAD	O4B-C1B-N9A-C8A
2	B	1250	NAD	O4B-C1B-N9A-C8A

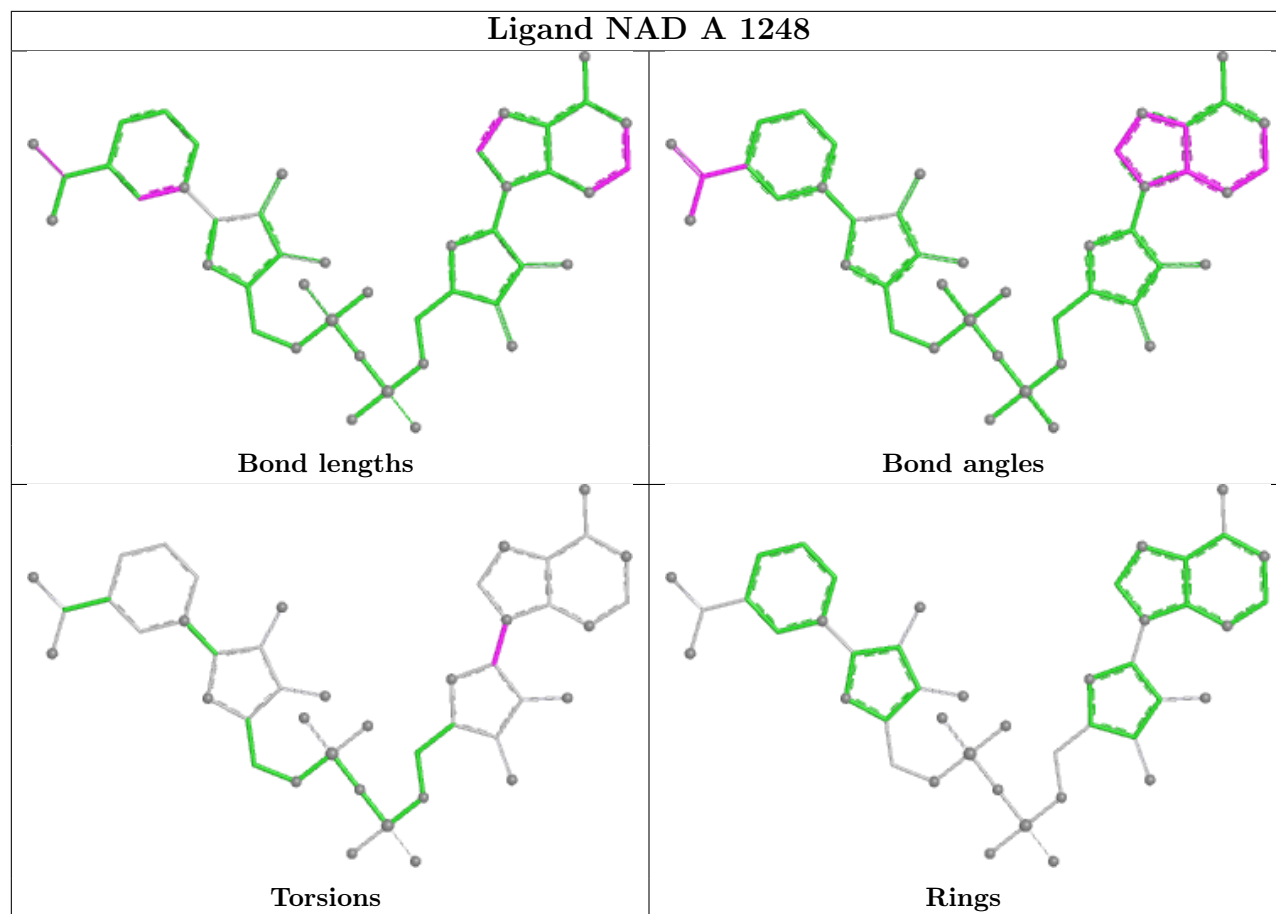
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	204/211 (96%)	0.54	15 (7%) 20 23	16, 25, 33, 35	1 (0%)
1	B	205/211 (97%)	1.22	48 (23%) 2 2	13, 29, 55, 65	5 (2%)
1	C	208/211 (98%)	1.18	47 (22%) 2 2	16, 27, 53, 59	2 (0%)
1	D	204/211 (96%)	1.01	36 (17%) 4 4	13, 28, 44, 51	2 (0%)
All	All	821/844 (97%)	0.99	146 (17%) 4 4	13, 27, 48, 65	10 (1%)

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	105	ILE	5.7
1	C	148	GLY	5.6
1	B	83	ALA	5.5
1	C	96	VAL	5.0
1	C	154	ALA	4.8
1	C	149	THR	4.8
1	C	183	PHE	4.7
1	C	97	ILE	4.7
1	D	105	ILE	4.7
1	A	245	GLY	4.7
1	D	103	ASN	4.6
1	C	92	GLN	4.6
1	C	150	ILE	4.6
1	C	146	SER	4.5
1	D	83	ALA	4.5
1	C	247	ALA	4.4
1	B	249	ASN	4.4
1	B	101	PRO	4.1
1	B	100	PHE	4.1
1	D	100	PHE	4.0
1	D	51	ASN	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	185	GLY	3.9
1	C	95	GLY	3.9
1	B	102	SER	3.8
1	B	99	GLY	3.8
1	C	234	GLY	3.8
1	B	97	ILE	3.8
1	A	247	ALA	3.8
1	C	151	ASN	3.7
1	B	98	ASN	3.7
1	C	248	ILE	3.7
1	D	183	PHE	3.6
1	A	140	GLN	3.5
1	B	90	LEU	3.5
1	B	45	THR	3.5
1	C	153	THR	3.5
1	B	107	GLN	3.5
1	B	248	ILE	3.4
1	A	44	ASN	3.4
1	C	93	ASN	3.4
1	D	96	VAL	3.4
1	B	96	VAL	3.4
1	B	103	ASN	3.3
1	C	143	LEU	3.3
1	C	139	PHE	3.3
1	D	245	GLY	3.3
1	B	50	THR	3.3
1	B	84	SER	3.2
1	B	93	ASN	3.2
1	C	230	LEU	3.2
1	C	44	ASN	3.2
1	C	145	ASN	3.2
1	C	45	THR	3.2
1	B	66	TYR	3.1
1	C	142	THR	3.1
1	B	46	TYR	3.1
1	D	85	GLU	3.1
1	B	52	ILE	3.1
1	C	147	ASN	3.0
1	A	244	MET	3.0
1	C	136	GLY	3.0
1	A	232	SER	2.9
1	D	97	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	244	MET	2.8
1	C	144	LEU	2.8
1	A	181	SER	2.8
1	B	71	SER	2.8
1	D	84	SER	2.8
1	B	104	LEU	2.8
1	B	88	GLY	2.8
1	C	184	ALA	2.7
1	C	133	ALA	2.7
1	C	155	PHE	2.7
1	D	78	SER	2.7
1	A	246	THR	2.7
1	B	95	GLY	2.7
1	C	245	GLY	2.6
1	D	53	ASP	2.6
1	C	231	SER	2.6
1	D	88	GLY	2.6
1	C	227	ASP	2.6
1	B	86	ILE	2.6
1	B	182	ALA	2.6
1	C	102	SER	2.6
1	D	247	ALA	2.6
1	D	98	ASN	2.6
1	D	99	GLY	2.6
1	C	157	LYS	2.6
1	A	57	ALA	2.6
1	D	44	ASN	2.6
1	D	101	PRO	2.6
1	C	233	ASP	2.5
1	D	95	GLY	2.5
1	D	92	GLN	2.5
1	B	69	SER	2.5
1	D	102	SER	2.5
1	B	63	TYR	2.5
1	D	227	ASP	2.5
1	D	106	LYS	2.5
1	C	137	THR	2.5
1	D	63	TYR	2.5
1	B	180	VAL	2.5
1	C	185	GLY	2.5
1	B	94	LYS	2.4
1	C	85	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	106	LYS	2.4
1	D	184	ALA	2.4
1	B	108	VAL	2.4
1	B	81	LYS	2.4
1	A	179	ASN	2.3
1	B	184	ALA	2.3
1	B	116	ASN	2.3
1	C	159	LYS	2.3
1	D	147	ASN	2.3
1	D	185	GLY	2.3
1	A	233	ASP	2.3
1	B	110	LEU	2.3
1	B	87	ASN	2.3
1	B	77	VAL	2.3
1	B	85	GLU	2.2
1	D	61	ALA	2.2
1	A	103	ASN	2.2
1	B	181	SER	2.2
1	B	227	ASP	2.2
1	C	100	PHE	2.2
1	B	92	GLN	2.2
1	D	232	SER	2.2
1	C	156	GLU	2.2
1	D	89	LYS	2.2
1	C	232	SER	2.2
1	A	92	GLN	2.2
1	D	67	GLY	2.2
1	C	98	ASN	2.2
1	B	170	TYR	2.2
1	C	101	PRO	2.2
1	A	185	GLY	2.1
1	A	230	LEU	2.1
1	B	53	ASP	2.1
1	B	61	ALA	2.1
1	B	68	LEU	2.1
1	D	52	ILE	2.1
1	D	54	GLN	2.1
1	C	105	ILE	2.1
1	B	78	SER	2.0
1	D	104	LEU	2.0
1	C	182	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

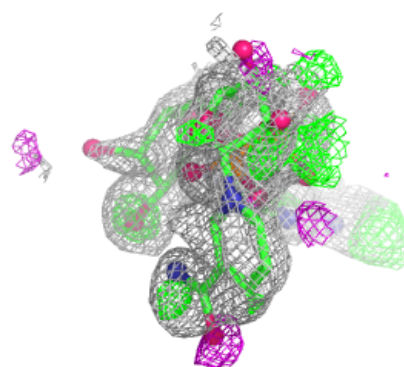
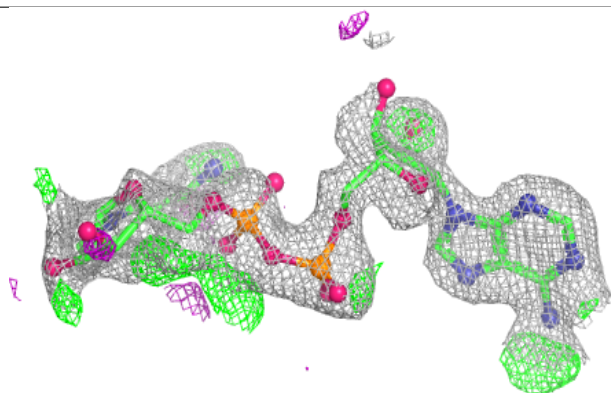
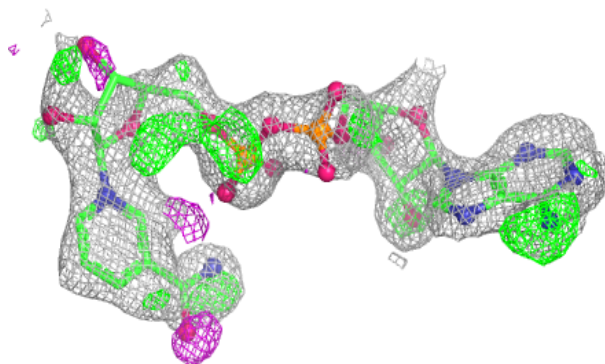
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	C	1252	5/5	0.69	0.21	39,39,39,39	5
2	NAD	B	1250	44/44	0.75	0.18	33,38,44,45	44
3	SO4	D	1248	5/5	0.86	0.23	34,34,35,35	5
3	SO4	D	1249	5/5	0.88	0.13	29,30,30,31	5
3	SO4	A	1250	5/5	0.89	0.11	35,35,36,37	5
3	SO4	B	1251	5/5	0.93	0.10	30,30,32,32	5
3	SO4	A	1249	5/5	0.94	0.08	30,31,32,32	5
2	NAD	A	1248	44/44	0.94	0.08	21,24,27,29	0

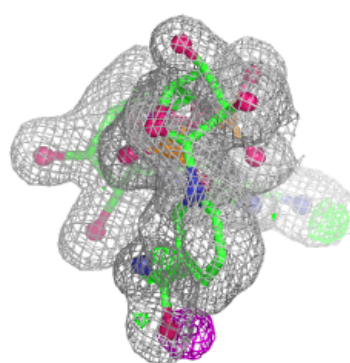
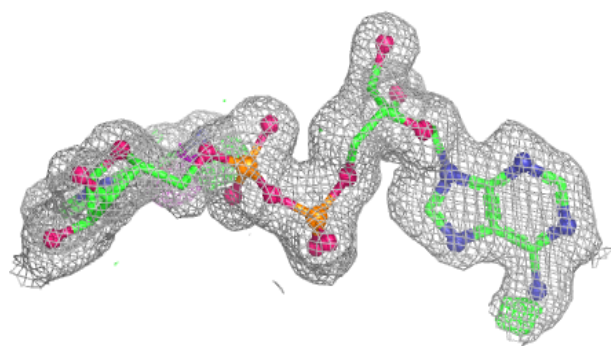
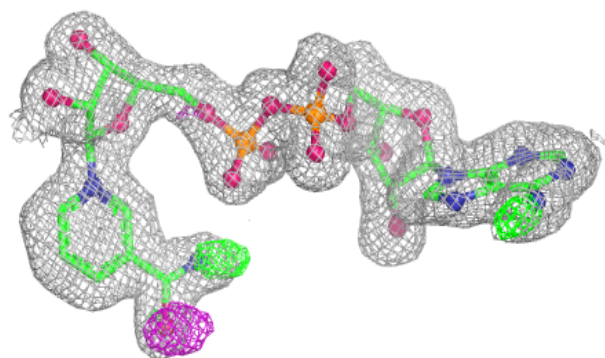
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NAD B 1250:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around NAD A 1248:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.